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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-7.02	-7.02

=> b reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	41.14	41.35
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-7.02	-7.02

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STRUCTURE FILE UPDATES: 14 NOV 2007 HIGHEST RN 953817-57-7  
DICTIONARY FILE UPDATES: 14 NOV 2007 HIGHEST RN 953817-57-7

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

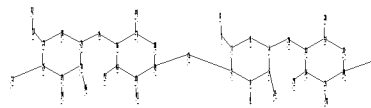
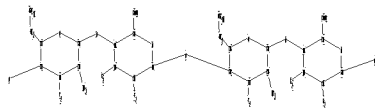
Please note that search-term pricing does apply when  
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predicted properties as well as tags indicating availability of  
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on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\jlau1\My Documents\10518303 - epiK5\free amine  
k5 structure - 2.str



chain nodes :

7 8 9 10 17 18 20 21 22 31 32 33 34 35 42 43 44 45 46

ring nodes :

1 2 3 4 5 6 11 12 13 14 15 16 25 26 27 28 29 30 36 37 38 39  
40 41

chain bonds :

1-9 2-45 3-7 5-10 6-22 7-8 10-11 12-20 14-21 15-18 16-17 25-34 26-33  
27-31 29-35 30-46 31-32 35-36 37-44 39-45 40-43 41-42

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 25-26  
25-30 26-27 27-28 28-29 29-30 36-37 36-41 37-38 38-39 39-40 40-41

exact/norm bonds :

1-2 1-6 1-9 2-3 2-45 3-4 4-5 5-6 5-10 6-22 10-11 11-12 11-16 12-13  
13-14 14-15 14-21 15-16 15-18 16-17 25-26 25-30 25-34 26-27 26-33 27-28  
28-29 29-30 29-35 30-46 35-36 36-37 36-41 37-38 38-39 39-40 39-45 40-41  
40-43 41-42

exact bonds :

3-7 7-8 12-20 27-31 31-32 37-44

G1:H, SO3H

G2:OH, OSO3H

Match level :

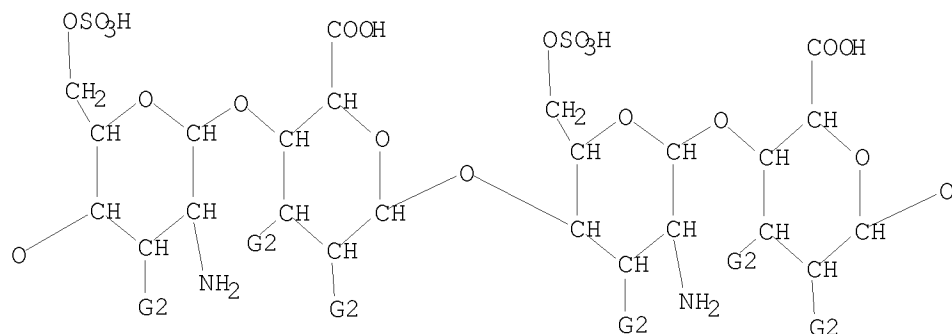
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11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 20:CLASS  
21:CLASS 22:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS  
32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:Atom 37:Atom 38:Atom 39:Atom  
40:Atom 41:Atom 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS

L6            STRUCTURE UPLOADED

=> d 16

L6 HAS NO ANSWERS

L6                            STR



G1 H, SO<sub>3</sub>H

G2 OH, OSO<sub>3</sub>H

Structure attributes must be viewed using STN Express query preparation.

=> s 16 sss sam

SAMPLE SEARCH INITIATED 08:23:22 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -            29 TO ITERATE

100.0% PROCESSED            29 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*

BATCH    \*\*COMPLETE\*\*

PROJECTED ITERATIONS:            257 TO            903

PROJECTED ANSWERS:                1 TO            80

L7                            1 SEA SSS SAM L6

=> d 17 scan

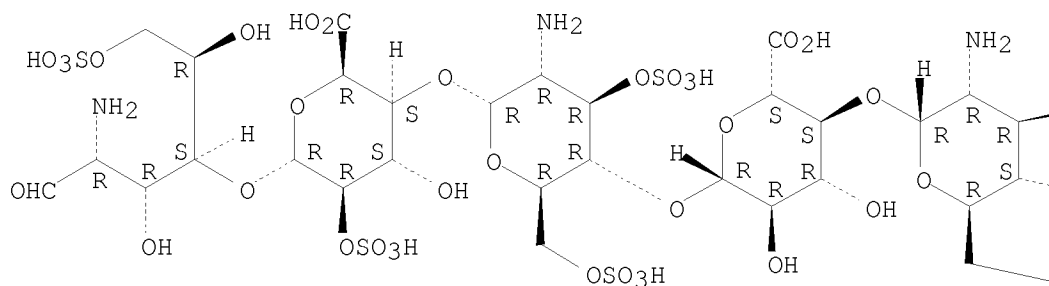
L7    1 ANSWERS    REGISTRY    COPYRIGHT 2007 ACS on STN

IN    D-Glucose, O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-  
      (1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-  
      3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2-O-sulfo- $\alpha$ -L-  
      idopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, 6-(hydrogen sulfate) (9CI)

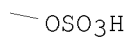
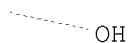
MF    C30 H51 N3 O40 S5

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s 16 sss full  
 FULL SEARCH INITIATED 08:23:54 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 760 TO ITERATE

100.0% PROCESSED 760 ITERATIONS 11 ANSWERS  
 SEARCH TIME: 00.00.01

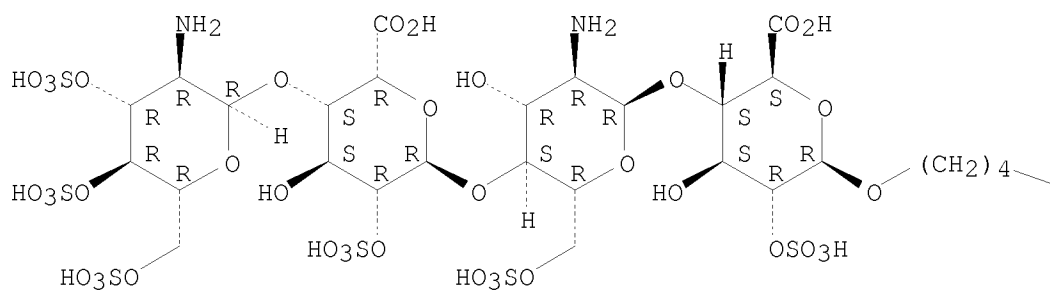
L8 11 SEA SSS FUL L6

=> d 18 scan

L8 11 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN  $\beta$ -D-Glucopyranosiduronic acid, pentyl O-2-amino-2-deoxy-3,4,6-tri-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-, 2-(hydrogen sulfate)  
 MF C29 H50 N2 O39 S6  
 CI COM

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

Me

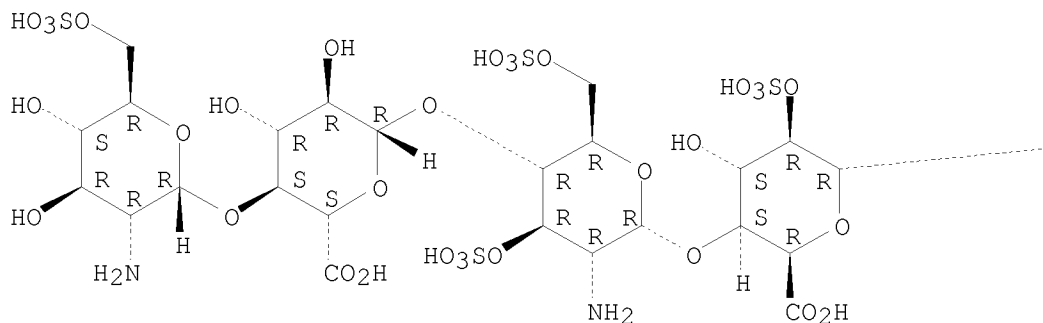
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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

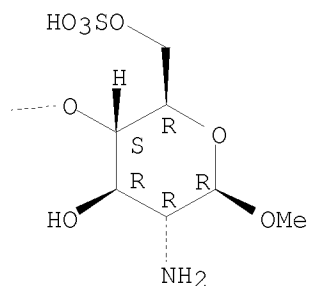
L8 11 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN β-D-Glucopyranoside, methyl O-2-amino-2-deoxy-6-O-sulfo-α-D-glucopyranosyl-(1→4)-O-β-D-glucopyranuronosyl-(1→4)-O-2-amino-2-deoxy-3,6-di-O-sulfo-α-D-glucopyranosyl-(1→4)-O-2-O-sulfo-α-L-idopyranuronosyl-(1→4)-2-amino-2-deoxy-,  
 6-(hydrogen sulfate), heptasodium salt (9CI)  
 MF C31 H53 N3 O40 S5 . 7 Na

Absolute stereochemistry.

PAGE 1-A



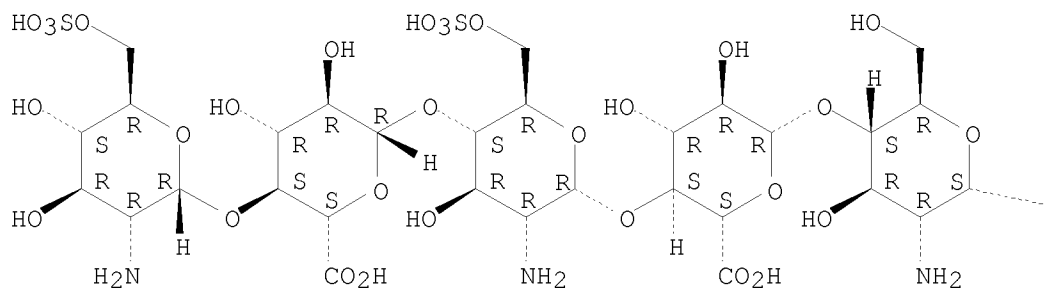
● 7 Na



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L8 11 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN  $\alpha$ -D-Glucopyranoside, methyl O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-  
 MF C31 H53 N3 O31 S2  
 CI COM

Absolute stereochemistry.



OMe

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	173.00	214.35
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-7.02

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 FILE LAST UPDATED: 14 Nov 2007 (20071114/ED)

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=> s 18

L9 8 L8

=> d 18 scan

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

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23955901 PY<=2003

L10 7 L9 AND PY<=2003

=> d 19 1-8 ibib abs hitstr

L9 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:921548 CAPLUS

DOCUMENT NUMBER: 142:89064

TITLE: Competing fragmentation processes in tandem mass spectra of heparin-like glycosaminoglycans

AUTHOR(S): Naggar, Estee F.; Costello, Catherine E.; Zaia, Joseph

CORPORATE SOURCE: Department of Biochemistry, Boston University School of Medicine, Boston, MA, USA

SOURCE: Journal of the American Society for Mass Spectrometry (2004), 15(11), 1534-1544

CODEN: JAMSEF; ISSN: 1044-0305

PUBLISHER: Elsevier Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Heparin-like glycosaminoglycans (HLGAGs) are highly sulfated, linear carbohydrates attached to proteoglycan core proteins and expressed on cell surfaces and in basement membranes. These carbohydrates bind several

families of growth factors and growth factor receptors and act as coreceptors for these mols. Tandem mass spectrometry has the potential to increase our understanding of the biol. significance of HLGAG expression by providing a facile means for sequencing these mols. without the need for time-consuming total purification. The challenge for tandem mass spectrometric anal. of HLGAGs is to produce abundant ions derived via glycosidic bond cleavages while minimizing the abundances of ions produced from elimination of the fragile sulfate groups. This work describes the competing fragmentation pathways that result from dissociation of high neg. charge state ions generated from HLGAGs. Glycosidic bond cleavage ion formation competes with losses of equivalent of H<sub>2</sub>SO<sub>4</sub>, resulting in complex ion patterns. For the most highly sulfated structure examined, an octasulfated tetramer, an unusual loss of charge from the precursor ion was observed, accompanied by low abundance ions originating from subsequent backbone cleavages. These results demonstrate that fragmentation processes competing with glycosidic bond cleavages are more favored for highly sulfated HLGAG ions. In conclusion, reduction of charge-charge repulsions, such as is achieved by pairing the HLGAG ions with metal cations, is necessary in order to minimize the abundances of ions derived via fragmentation processes that compete with glycosidic bond cleavages.

IT 525593-68-4

RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)

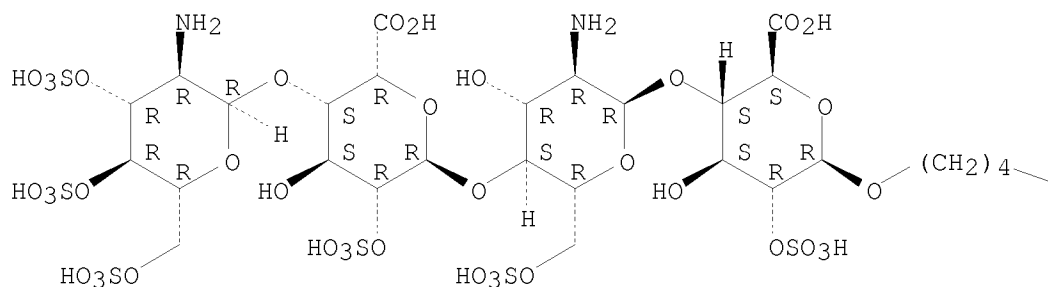
(competing fragmentation processes in tandem mass spectra of heparin-like glycosaminoglycans)

RN 525593-68-4 CAPLUS

CN  $\beta$ -D-Glucopyranosiduronic acid, pentyl O-2-amino-2-deoxy-3,4,6-tri-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-, 2-(hydrogen sulfate) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

Me

REFERENCE COUNT:

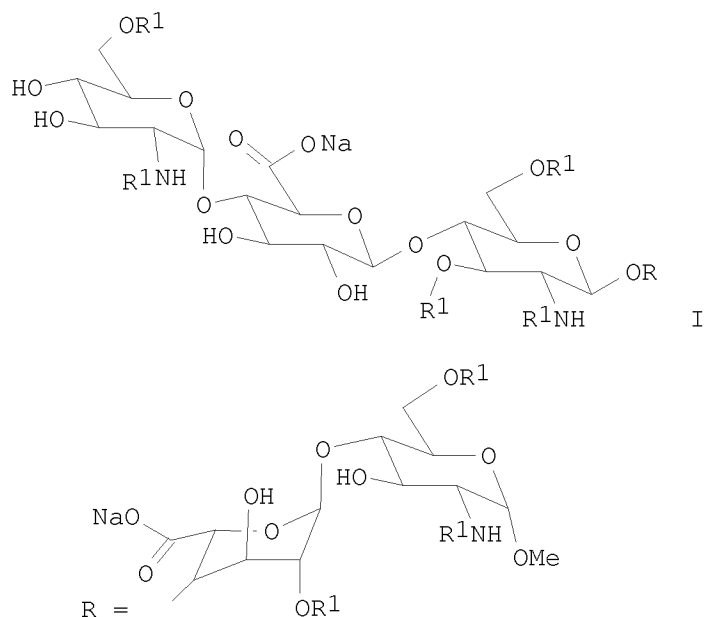
34

THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



ACCESSION NUMBER: 2003:221700 CAPLUS  
 DOCUMENT NUMBER: 138:221788  
 TITLE: Synthetic heparin pentasaccharides via glycosylation reaction using different protecting groups  
 INVENTOR(S): Seifert, Joachim; Singh, Latika; Ramsdale, Tracie Elizabeth; West, Michael Leo; Drinnan, Nicholas Barry  
 PATENT ASSIGNEE(S): Alchemia Pty Ltd., Australia  
 SOURCE: PCT Int. Appl., 207 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003022860	A1	20030320	WO 2002-AU1228	20020906
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2459562	A1	20030320	CA 2002-2459562	20020906
AU 2002331426	A1	20030324	AU 2002-331426	20020906
EP 1440077	A1	20040728	EP 2002-766941	20020906
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1558911	A	20041229	CN 2002-821855	20020906
JP 2005505565	T	20050224	JP 2003-526933	20020906
US 2005080042	A1	20050414	US 2004-488677	20040930
AU 2007203325	A1	20070809	AU 2007-203325	20070718
PRIORITY APPLN. INFO.:			AU 2001-7587	A 20010907
			AU 2002-331426	A3 20020906
			WO 2002-AU1228	W 20020906
OTHER SOURCE(S):		MARPAT 138:221788		
GI				



AB Synthetic monosaccharides, disaccharides, trisaccharides, tetrasaccharides and pentasaccharides for use in the preparation of synthetic heparinoids. Thus, heparin pentasaccharide I ( $R_1 = \text{SO}_3\text{Na}$ ) was prepared via glycosylation reaction using different protecting groups.

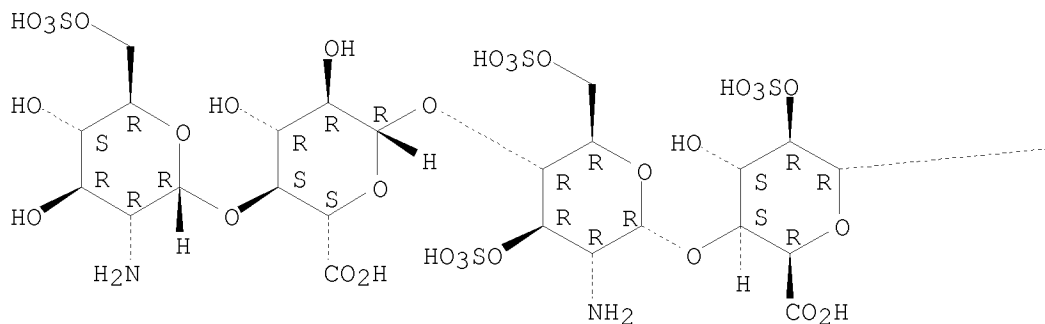
IT 114870-02-9P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthetic heparin pentasaccharides via glycosylation reaction using different protecting groups)

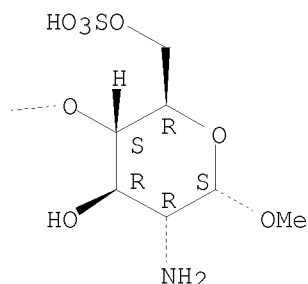
RN 114870-02-9 CAPLUS

CN  $\alpha$ -D-Glucopyranoside, methyl O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, 6-(hydrogen sulfate), heptasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:69762 CAPLUS

DOCUMENT NUMBER: 138:385647

TITLE: Modular synthesis of heparin oligosaccharides

AUTHOR(S): Orgueira, Hernan A.; Bartolozzi, Alessandra; Schell, Peter; Litjens, Remy E. J. N.; Palmacci, Emma R.; Seeberger, Peter H.

CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Chemistry--A European Journal (2003), 9(1), 140-169  
CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:385647

AB A general, modular strategy for the first completely stereoselective synthesis of defined heparin oligosaccharides is described. Six monosaccharide building blocks (four differentially protected glucosamines, one glucuronic and one iduronic acid) were utilized to prepare di- and trisaccharide modules in a fully selective fashion. Installation of the  $\alpha$ -glucosamine linkage was controlled by placing a conformational constraint on the uronic acid glycosyl acceptors thereby establishing a new concept for stereochem. control. Combination of disaccharide modules to form trans-uronic acid linkages was completely selective by virtue of C2 participating groups. Coupling reactions between disaccharide modules exhibited sequence dependence. While the union of many glucosamine uronic acid disaccharide modules did not meet any problems, certain sequences proved not accessible. Elaboration of glucosamine uronic acid disaccharide building blocks to trisaccharide modules by addition of either one addnl. glucosamine or uronic acid allowed for stereoselective access to oligosaccharides as demonstrated on the example of a hexasaccharide resembling the ATIII-binding sequence. Final deprotection and sulfation yielded the fully synthetic heparin oligosaccharides.

IT 525593-68-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heparin oligosaccharides using modular synthesis techniques)

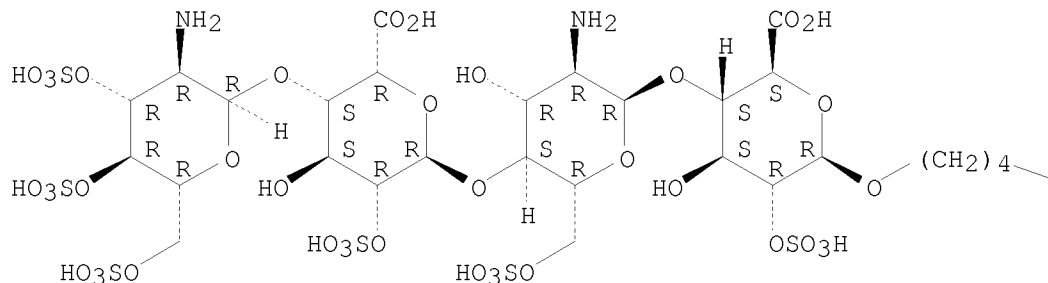
RN 525593-68-4 CAPLUS

CN  $\beta$ -D-Glucopyranosiduronic acid, pentyl O-2-amino-2-deoxy-3,4,6-tri-O-

sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-, 2-(hydrogen sulfate) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

Me

REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

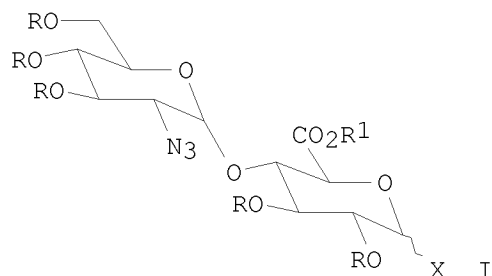
L9 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2002:574867 CAPLUS  
 DOCUMENT NUMBER: 137:125357  
 TITLE: Solid- and solution-phase combinatorial libraries  
 synthesis of heparin and other glycosaminoglycans as  
 potential receptors  
 INVENTOR(S): Seeberger, Peter H.; Orgueira, Hernan; Schell, Peter  
 PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA  
 SOURCE: PCT Int. Appl., 131 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002058633	A2	20020801	WO 2002-US1772	20020122
WO 2002058633	A3	20021017		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2435637	A1	20020801	CA 2002-2435637	20020122
AU 2002243630	A1	20020806	AU 2002-243630	20020122
US 2003013862	A1	20030116	US 2002-54724	20020122
US 6846917	B2	20050125		
EP 1353556	A2	20031022	EP 2002-709129	20020122
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US 2005187381	A1	20050825	US 2005-40834	20050121
PRIORITY APPLN. INFO.:			US 2001-263621P	P 20010123
			US 2002-54724	A1 20020122
			WO 2002-US1772	W 20020122
OTHER SOURCE(S):			MARPAT 137:125357	
GI				



AB Described is a modular, general synthetic strategy for the preparation in solution and on a solid support of heparin, heparin-like glycosaminoglycans, glycosaminoglycans and non-natural analogs, e.g. I, wherein X is OH, acyloxy, silyloxy, halide, alkylthio, arylthio, alkoxy, OC(NH)CCl<sub>3</sub>; R is H, alkyl, aryl, arylalkyl, heteroarylalkyl, silyl, acyl, alkenyloxycarbonyl, aralkyloxycarbonyl; R<sub>1</sub> is H, alkyl, aryl, arylalkyl, heteroarylalkyl and derivs. Addnl., the modular strategy provides the basis for the preparation of combinatorial libraries and parallel libraries of defined glycosaminoglycan oligosaccharides. The defined glycosaminoglycan structures may be used in high-throughput screening expts. to identify carbohydrate sequences that regulate a host of recognition and signal-transduction processes. The determination of specific sequences involved in receptor binding holds great promise for the development of mol. tools which will allow modulation of processes underlying viral entry, angiogenesis, kidney diseases and diseases of the control nervous system (no data). Notably, the present invention enables the automated synthesis of glycosaminoglycans in much the same fashion that peptides and oligonucleotides are currently assembled. Thus, n-pentenyl (2-deoxy-2-sodium sulfonatamido-3,4,6-tri-O-sodium sulfonato- $\alpha$ -D-glucopyranosyl)-(1 $\rightarrow$ 4)-(sodium 2-O-sodium sulfonato- $\alpha$ -D-idopyranosyluronate)-(1 $\rightarrow$ 4)-(2-deoxy-2-sodium sulfonatamido-6-O-sodium sulfonato- $\alpha$ -D-glucopyranosyl)-(1 $\rightarrow$ 4)-sodium 2-O-sodium sulfonato- $\beta$ -D-glucopyranosiduronate was prepared as potential receptors.

IT 444119-15-7P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (solid-phase combinatorial libraries synthesis of glycosaminoglycans as potential receptors)

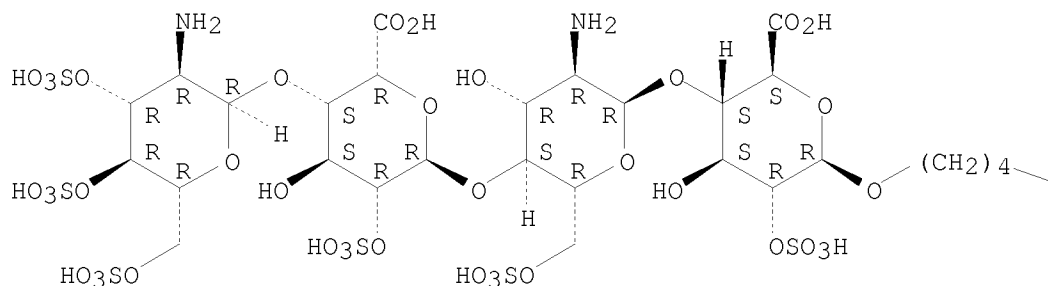
RN 444119-15-7 CAPLUS

CN  $\beta$ -D-Glucopyranosiduronic acid, pentyl O-2-amino-2-deoxy-3,4,6-tri-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2-O-sulfo- $\alpha$ -L-

idopyranuronosyl-(1→4)-O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1→4)-, 2-(hydrogen sulfate), octasodium salt (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

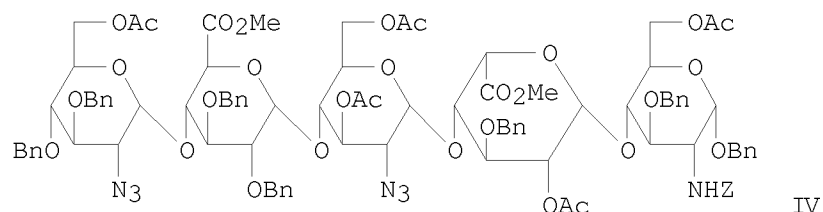
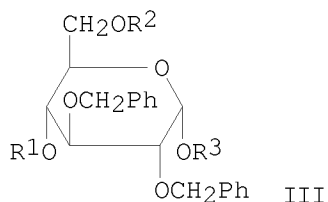
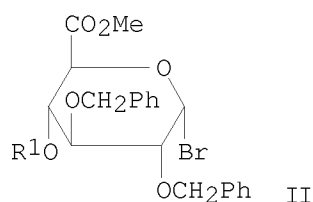
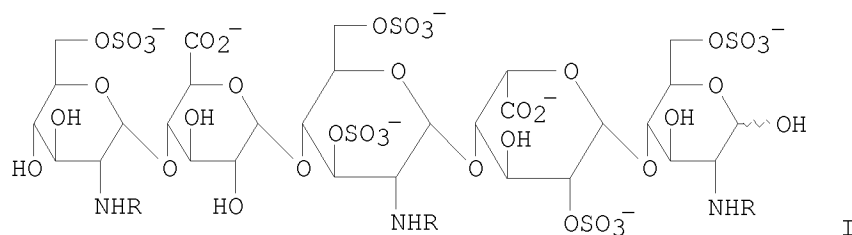


● 8 Na

PAGE 1-B

Me

L9 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1990:198939 CAPLUS  
 DOCUMENT NUMBER: 112:198939  
 TITLE: Synthesis of an N-acetylated heparin pentasaccharide and its anticoagulant activity in comparison with the heparin pentasaccharide with high anti-factor-Xa activity  
 AUTHOR(S): Wessel, Hans Peter; Labler, Ludvik; Tschopp, Thomas B.  
 CORPORATE SOURCE: Pharm. Res. Dep., F. Hoffmann-La Roche A.-G., Basel, CH-4002, Switz.  
 SOURCE: Helvetica Chimica Acta (1989), 72(6), 1268-77  
 CODEN: HCACAV; ISSN: 0018-019X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 112:198939  
 GI



AB The synthesis of heparin pentasaccharide (I; R = Ac) is described. It was assembled from 5 suitably block monosaccharide units. Glucuronic acid building block II (R1 = levulinoyl) was prepared from glucose by direct Jones oxidation of 6-O-trityl derivative III (R1 = levulinoyl, R2 = trityl, R3 =

= allyl). The resulting acid was esterified in large amts. using ClCO2Me/base. Me3SiBr proved to be an excellent reagent for the hydrolysis of the prop-1-enyl glycoside. The pentasaccharide IV (Bn = PhCH2) was obtained by a [2+2]+1 synthesis; the glycosylations furnished good to very good yields. The identity of protected oligosaccharides was confirmed by 1H-NMR. Sequential deblocking of the pentasaccharide, O-sulfation, and N-acetylation gave I (R = Ac) which was shown to exhibit .apprx.600 times lower anticoagulant activity than I (R = SO3-).

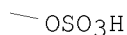
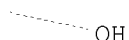
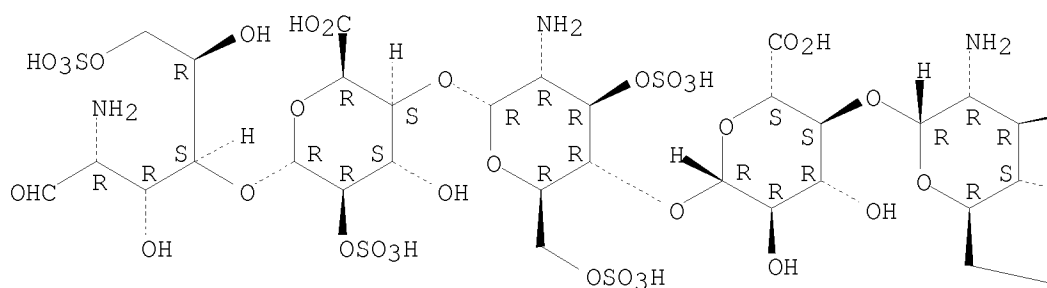
IT 126684-11-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and acetylation of)

RN 126684-11-5 CAPLUS

CN D-Glucose, O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, 6-(hydrogen sulfate) (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:574547 CAPLUS

DOCUMENT NUMBER: 111:174547

TITLE: Synthesis of several sulfated and nonsulfated pentasaccharides, corresponding to the E. coli K5 glycosaminoglycan

AUTHOR(S): Kraaijeveld, N. A.; Van Boeckel, C. A. A.

CORPORATE SOURCE: Sci. Dev. Group, Organon Int. B.V., Oss, 5340 BH, Neth.

SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1989), 108(2), 39-50

CODEN: RTCPA3; ISSN: 0165-0513

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:174547

AB The synthesis of 4 pentasaccharides, which are structurally related to the bacterial capsular polysaccharide isolated from Escherichia coli K5 (010/K5/H40), i.e. the so-called K5 antigen, is described. These 4 synthetic compds. comprise a pentasaccharide that is structurally identical to the K5 antigen, 2 pentasaccharides containing 2 and 3 O-sulfated groups, resp., and a pentasaccharide that is O-sulfated on all hydroxy groups. These 4 K5-antigen-related pentasaccharides were synthesized from fully protected pentasaccharides, which were prepared by conventional methods. Structural assignments of the K5-antigen-related pentamers were confirmed by <sup>1</sup>H and <sup>13</sup>C NMR.

IT 122992-71-6P 122992-73-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and N-acetylation of)

RN 122992-71-6 CAPLUS

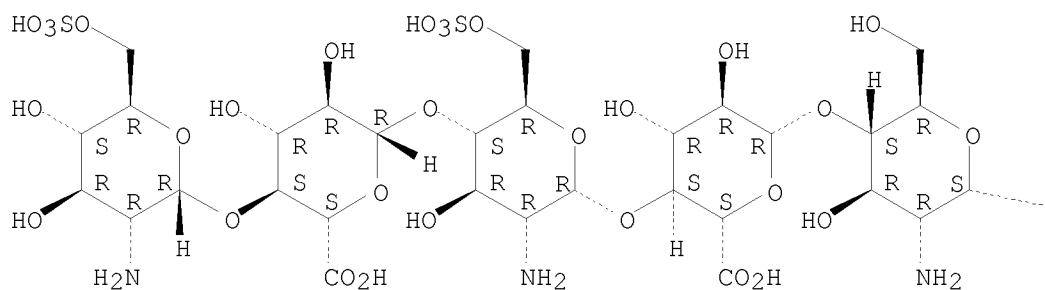
CN α-D-Glucopyranoside, methyl O-2-amino-2-deoxy-6-O-sulfo-α-D-glucopyranosyl-(1→4)-O-β-D-glucopyranuronosyl-(1→4)-O-2-



amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, tetrasodium salt (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



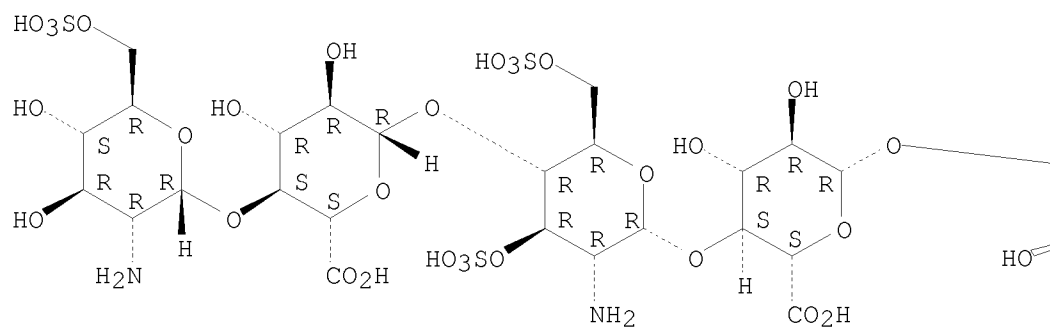
● 4 Na

PAGE 1-B

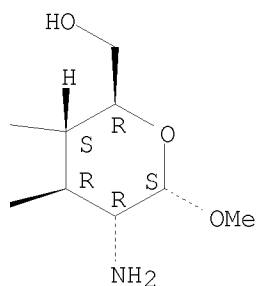
OMe

RN 122992-73-8 CAPLUS  
CN  $\alpha$ -D-Glucopyranoside, methyl O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, pentasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● 5 Na



L9 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1989:115268 CAPLUS  
 DOCUMENT NUMBER: 110:115268  
 TITLE: Preparation of a fragment of mucopolysaccharide  
 heparin as an anticoagulant and antithrombotic  
 INVENTOR(S): Kuzuhara, Hiromi; Ichikawa, Yukitaka; Kasama, Toshio;  
 Iwata, Yoshinori; Kadota, Ryuji  
 PATENT ASSIGNEE(S): Institute of Physical and Chemical Research, Japan;  
 Kodama, Ltd.  
 SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63218691	A	19880912	JP 1987-53401	19870309
PRIORITY APPLN. INFO.: GI			JP 1987-53401	19870309

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title pentasaccharide (I; R = NHSO<sub>3</sub>Na, R<sub>1</sub> = R<sub>2</sub> = SO<sub>3</sub>Na, R<sub>3</sub> = H, R<sub>4</sub> = Na) (II), useful as an anticoagulant and an antithrombotic, was prepared Glycosidation of a tetrasaccharide III with 6-O-acetyl-2-azido-3,4-di-O-benzyl- $\alpha$ -D-glucopyranosyl bromide (IV) in ClCH<sub>2</sub>CH<sub>2</sub>Cl in the presence of CF<sub>3</sub>SO<sub>3</sub>Ag, mol. sieves 4A, and 2,4,6-collidine at -15° gave 77% I (R = N<sub>3</sub>, R<sub>1</sub> = Ac, R<sub>2</sub> = Bz, R<sub>3</sub> = CH<sub>2</sub>Ph, R<sub>4</sub> = Me) which was saponified with 5N aqueous NaOH and aqueous MeOH and then reesterified with diazomethane to give

58%

I (R = N<sub>3</sub>, R<sub>1</sub> = R<sub>2</sub> = H, R<sub>3</sub> = CH<sub>2</sub>Ph, R<sub>4</sub> = Me). Sulfation of the latter compound with SO<sub>3</sub>.Et<sub>3</sub>N in DMF and purification of the product by a Sephadex

LH-20

column followed by treatment with SP Sephadex C-25 (Na<sup>+</sup> type) gave 80% I (R = N<sub>3</sub>, R<sub>1</sub> = R<sub>2</sub> = SO<sub>3</sub>Na, R<sub>3</sub> = CH<sub>2</sub>Ph, R<sub>4</sub> = Me). Hydrogenation of the latter over 10% Pd/C in aqueous MeOH and sulfation of the resulting I (R = NH<sub>2</sub>, R<sub>1</sub> = R<sub>2</sub> = SO<sub>3</sub>Na, R<sub>3</sub> = H, R<sub>4</sub> = Me) with SO<sub>3</sub>.Et<sub>3</sub>N followed by saponification with aqueous NaOH, purification by a Sephadex G-25 (equilibrated with 0.2M

aqueous

NaCl) and treatment with Dowex AG1-X2 (equilibrated with 0.5M aqueous NaCl) gave 16% II. II inhibited CaCl<sub>2</sub>-induced coagulation of sheep blood plasma with 60 U/mg vs. 155 U/mg for heparin. An injection formulation containing II 15, NaHCO<sub>3</sub> 0.2, NaCl 0.4 g, and H<sub>2</sub>O 100 mL was described.

IT 119254-84-1P

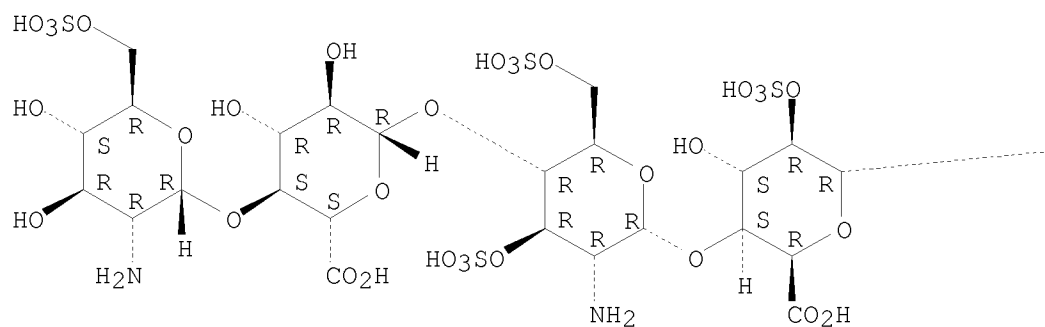
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as anticoagulant and antithrombotic)

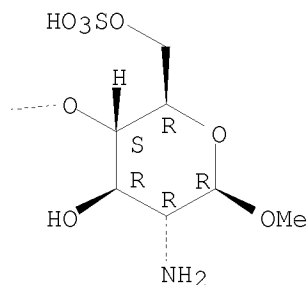
RN 119254-84-1 CAPLUS

CN  $\beta$ -D-Glucopyranoside, methyl 0-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, 6-(hydrogen sulfate), heptasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





L9 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:423222 CAPLUS

DOCUMENT NUMBER: 109:23222

TITLE: Synthesis of heparin fragments: a methyl  $\alpha$ -pentaoside with high affinity for antithrombin III

AUTHOR(S): Petitou, Maurice; Duchaussoy, Philippe; Lederman, Isidore; Choay, Jean; Jacquinet, Jean Claude; Sinay, Pierre; Torri, Giangiacomo

CORPORATE SOURCE: Inst. Choay, Paris, 75782, Fr.

SOURCE: Carbohydrate Research (1987), 167, 67-75

CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:23222

GI For diagram(s), see printed CA Issue.

AB The synthesis is described of the Me  $\alpha$ -glycoside, I (R = Me), of pentasaccharide I (R = H) which represents the sequence in heparin responsible for binding and activation of the anticoagulant protein Antithrombin III. It was obtained in a yield much better than that of the previously synthesized pentasaccharide and exhibited the same biol. properties.

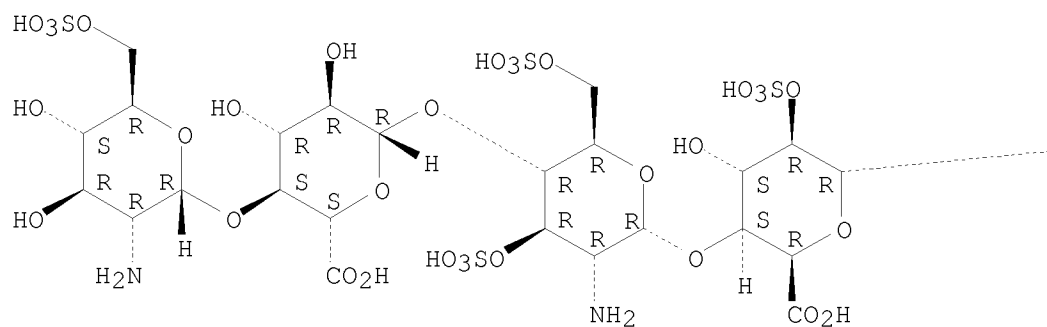
IT 114870-02-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and N-sulfation of)

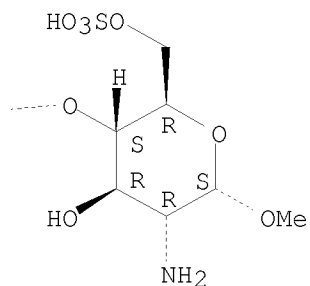
RN 114870-02-9 CAPLUS

CN  $\alpha$ -D-Glucopyranoside, methyl O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, 6-(hydrogen sulfate), heptasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● 7 Na



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COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
45.11	259.46
SINCE FILE	TOTAL
ENTRY	SESSION
-6.24	-13.26

SESSION WILL BE HELD FOR 120 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 08:25:43 ON 15 NOV 2007